



Modeling of thermal stresses in a microtubular Solid Oxide Fuel Cell stack



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HIGHLIGHTS

- No cracking of anode and electrolyte was predicted for temperatures lower than 750 °C at the voltage of 0.7 V.
- Risk of cracking damage for the cathode layer was confirmed for working temperature of 750 °C at the voltage of 0.7 V.
- The largest total axial stress of 212 MPa was found for cathodes of the fuel cells at the outer row.

ARTICLE INFO

Article history:

Received 16 February 2015

Received in revised form

9 September 2015

Accepted 11 September 2015

Available online 22 September 2015

Keywords:

Computational fluid dynamics (CFD)

Finite element method (FEM)

Microtubular Solid Oxide Fuel Cell (mSOFC) stack

Thermal stresses

ABSTRACT

A modeling study was carried out to analyze thermal stresses in a microtubular Solid Oxide Fuel Cell (mSOFC) stack and to estimate thermal expansion of the fuel cells inside the stack. A joint analysis by Computational Fluid Dynamics (CFD) and Computational Structural Mechanics Finite Element Method (FEM) was performed. Temperature profiles generated by the thermo-hydrodynamic model were applied in the thermo-mechanical model to calculate thermal stress distributions in the mSOFC stack. The results yield maximum thermal axial elongation equal to 1.34 mm for the mSOFC stack, while the maximum radial elongation was equal to 0.496 mm. Modeled maximum equivalent (von Mises) stress was equal to 538 MPa in the contact areas of the cylindrical housing and manifold on the fuel inlet side. Based on comparison of the total axial stresses and the residual ones with the material strength it was noticed that the anode and electrolyte layers should not be critically deformed, but there is a risk of damage for cathode layers at chosen fuel cell configurations. A high risk of damage was also noticed for the outer housing, near contact points with manifolds as well as at the air distributor due to large number of cut-outs in the material.

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1. Introduction

The major limitation to mSOFC lifetime comes from the degradation of its component materials, which results from operating mSOFC at elevated temperatures. High temperatures give rise to significant thermal stresses mainly due to mismatch of thermal expansion coefficients of the cell components as well as temperature gradients in the fuel cell [1]. Thermal stresses may also cause microstructural instability and sub-critical cracking [2]. In addition, stack degradation tends to be faster than fuel cell degradation as a consequence of interconnect contact degradation [3,4]. Moreover, gas tightness of a mSOFC stack can also affect thermo-electrochemical behavior of the stack and degrade its performance or

even could lead to its damage in a long term operation [5].

Numerous numerical simulation models have been developed for planar and tubular SOFC designs to investigate thermal stresses in fuel cell components [6–8] and to predict the behavior of sealants [1,2,5,9,10]. For planar SOFC stack, Lin et al. (2007) [1] as the first incorporated a glass-ceramic sealant into a 3D Finite Element Analysis (FEA) model to produce more realistic results in thermal stress analysis and enhance the reliability of prediction of potential failure locations in the stack. The effects of stack support conditions, temperature gradients and thermal expansion mismatch between components were characterized. The modeling results indicated that thermal stress distribution did not differ significantly in each unit fuel cell of the planar SOFC stack, while the thermal expansion behavior of the metallic interconnect/frame had a greater influence on thermal distributions in a positive electrode-electrolyte-negative electrode (PEN) assembly [1]. More recently studies focus on the

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transient thermomechanical behavior of planar SOFCs [2,11–14]. A coupled Computational Fluid Dynamics (CFD) and Computational Structural Mechanics analysis was performed by Peksen et al. (2013) [2] for a full scale planar SOFC short stack over a whole thermal cycle. Cell components, wire-mesh, metal frame, interconnector plates and sealant materials were considered in the model. Thermomechanical behavior of the fuel cell stack during the heating-up, start-up and the shut-down stages were analyzed and major sources causing thermo-mechanically induced stress were defined. The simulations indicated that the stress during initial stages of the heating-up phase was the most critical during an operating cycle of the stack. Thermomechanical behavior of the sealant materials was triggered mostly by displacement of the steel components. On the other hand, the cooling stage results implied that the thermo-mechanical stress was driven by elastic behavior of the steel components. The main source of thermal strain was temperature difference between the local temperature and the initial stress free temperature that had been specified at 800 [°C] [2]. Thermal stress distributions in a new design of a hexagonal stack consisting of planar anode-supported Solid Oxide Fuel Cells was also examined by Wei, Wang & Wu (2014) [14]. The material of the cell support was Grancrete. Simulations were based on coupling the FLUENT flow solver with SOFC module and ANSYS stress solver. The flow solver provides species and temperature distributions to the SOFC module, while temperature distribution results of the next step of calculations were used in the ANSYS stress solver to calculate the induced stress. The stress modeling included the von Mises stress in metal and the maximum principal stress in ceramic material. The results revealed that the use of Grancrete cell support effectively reduced the maximum principal stress of the fuel cell and that the simulated maximum von Mises stress was 342 MPa, which was lower than the yield strength of stainless steel of 363 MPa [14]. These simulations delivered a proof that it is possible to optimize construction of a fuel cell stack based on numerical models at a lower cost in comparison to experiments, which are based on a trial-and-error approach.

In parallel, numerical investigations of a tubular SOFC design were carried out. Nakajo et al. (2006) [6] performed a sensitivity analysis of the stresses resulting from the mismatch between the layer coefficients of thermal expansion in order to provide guidelines for mechanical requirements and choice of SOFC materials. Their CFD results revealed that the stress magnitude was higher at the fuel/air inlet, where the internal steam reforming reactions induce a temperature drop. The greatest difference between the actual temperature and the sintering temperature occurred when the cell was at room temperature. However, that study neglected interactions between fuel cells and the other components such as sealants and therefore do not represent the actual stress field in fuel cell operation. The most rigorous study on thermal stresses analysis in an operating micro-tubular Solid Oxide Fuel Cell was done by Serincan, Pasaogullari & Sammes (2010) [11], in which thermal stresses arising from fabrication of the cell, exterior constraints and fuel cell operation were analyzed. The stresses were calculated based on a temperature field obtained from previously developed thermal-fluid model [12]. Serincan, Pasaogullari & Sammes (2010) [11] distinguished the following effects of factors determining stress distribution in fuel cell components: residual stresses, exterior stress loading due to the interactions with peripherals, temperature gradients presented during the fuel cell operation as well as effects of oxygen vacancies in the ceria based electrolyte. Simulations were done in a commercial multi-physics software COMSOL, which had capability of coupling a thermo-fluid model with a solid mechanics model into a single model. This coupling enabled to predict temperature field, which affects the stress distribution in the solid mechanics model. The authors [11] found out that stress distribution near a fuel cell–sealant interface changes significantly,

while the spatial temperature gradient had a minimal impact on the stress distribution for typical fuel cell operation at mid-range current densities. In addition, it was noticed that stresses in electrolyte decreased with introduction of oxygen vacancies in Gadolinia-Doped Ceria (GDC).

Numerical modeling is essential to study thermal stresses distributions in Solid Oxide Fuel Cell stack, since a SOFC stack has a complex design and is tightly sealed. Thus, it is hard to get experimental information such as spatial temperature gradients, which have significant impact on the stress distribution inside stack. Therefore, it is cost effective and time saving if the numerical modeling can support development of a new SOFC stack design and help researchers to gain a better understanding of the complex multiphysical processes taking place inside fuel cells and the SOFC stack. For this purpose, we present a detailed mechanical analysis of a new design of the microtubular Solid Oxide Fuel Cell stack consisting of 48 anode-supported fuel cells distributed over the circumference in four rows. The interactions between fuel cells, manifolds providing sealants, cylindrical housing, internal cylindrical air distributor as well as internal and external rings are accounted for a better representation of the current SOFC stack design. We analyze the residual stresses induced in the anode–electrolyte–cathode layers as two-stage cooling process of the sintered fuel cell layers. The effect of spatial temperature gradient on the stress distribution in the SOFC stack is also analyzed. In addition, the radial and axial displacement of the assembly with supporting structure under thermal stresses is estimated. Furthermore, the influence of temperature nonuniformity among fuel cells and the SOFC stack with supporting structure on axial stress distributions is studied. The numerical results will be used to determine areas of high values of stresses, which are higher than the yield strength of materials. The FEM results can be applied as the guide for possible construction optimization of the microtubular SOFC stack.

2. Mathematical model

2.1. Thermo-fluid model

In the first modeling step, Computational Fluid Dynamics (CFD) simulations of a microtubular Solid Oxide Fuel Cell stack were performed. The commercial CFD package ANSYS – FLUENT was used to model the thermal-fluid fields. The second step comprised a Computational Structural Mechanics (CSM) analysis based on Finite Element Method (FEM) to predict thermal stress distribution within a fuel cell stack using the commercial software ANSYS Mechanical. The flow solver delivers temperature distributions to the stress solver. Based on a temperature distribution, stress distribution including the von Mises (equivalent) stress in ceramic material were derived. The thermo-fluid model consists of the conservation of mass, momentum and energy equations, assuming a stationary incompressible laminar flow accompanied by heat transfer at the Reynolds number equal to 13.94:

$$\nabla(\rho\bar{u}) = 0 \quad (1)$$

$$(\rho\bar{u} \cdot \nabla)\bar{u} = -\nabla p + \nabla \cdot \left[\mu \left(\nabla\bar{u} + (\nabla\bar{u})^T \right) - \frac{2}{3} \mu \nabla \cdot \bar{u} \right] + \rho\bar{g} \quad (2)$$

where:

- \bar{g} is the acceleration due to gravity,
- p is the static pressure,
- ρ is the density of air,
- μ is the air dynamic viscosity,
- \bar{u} is the velocity vector,

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